# *High-frequency cavity modes: efficient computation and applications*

NJIT, February 7, 2005

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Thanks to J. Goodman, L. Greengard, P. Deift, P. Sarnak (NYU), H. Tureci (Yale), . . .

# Dirichlet eigenproblem

Normal modes of elastic membrane or 'drum' (Germain, Helmholtz, $19^{th}$C)
Eigenfunctions $\phi_j$ of Laplacian $\Delta$ in bounded domain $\Omega \subset \mathbb{R}^d$

$$-\Delta\phi_j = E_j\phi_j, \qquad \phi_j|_{\partial\Omega} = 0 \qquad \int_\Omega \phi_i\phi_j = \delta_{ij}$$

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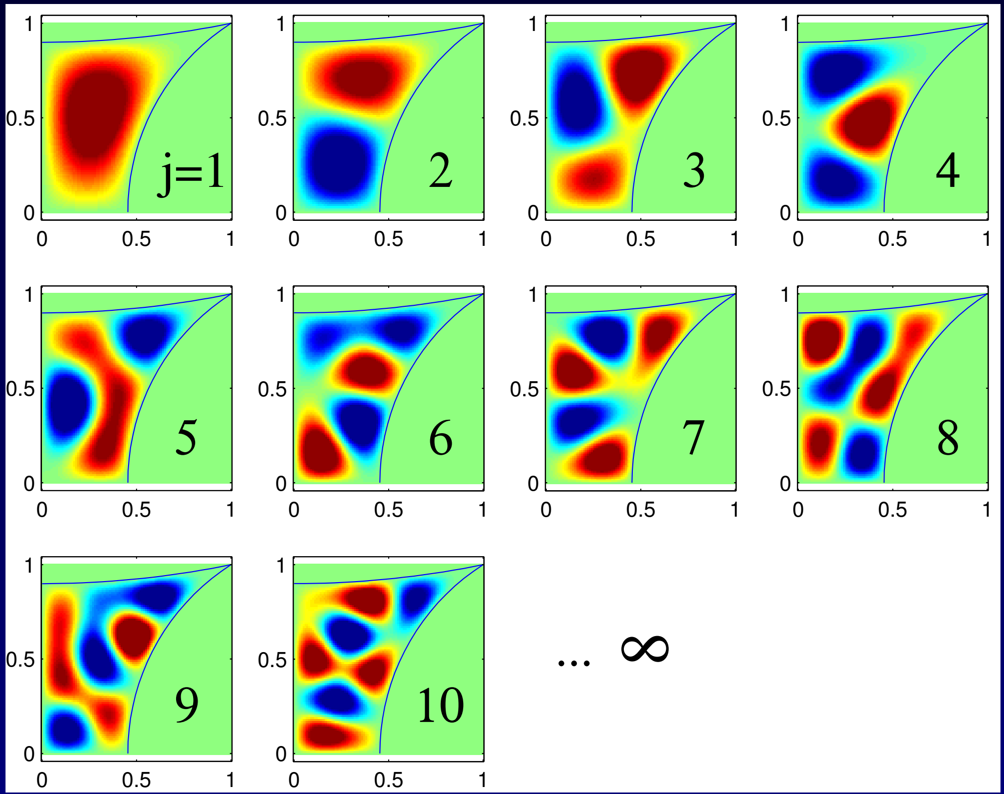


'level' $j = 1 \cdots \infty$

'energy' eigenvalue $E_j$

wavenumber $k_j = E_j^{1/2}$

wavelength $= 2\pi/k_j$

focus on $d$=2

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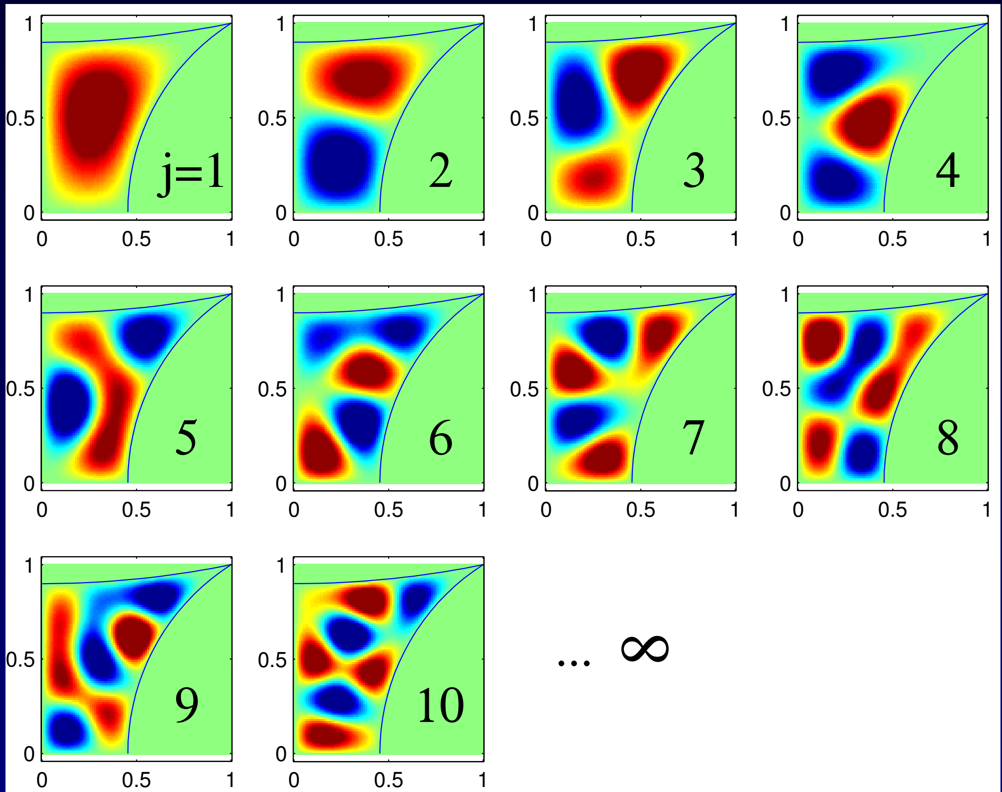


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- Analytic solutions only when $\Delta$ separable (rectangle, ellipse…)
- How numerically compute large numbers of $E_j$ & $\phi_j$ efficiently?

# Motivation

- electromagnetic waveguides (TM modes: Dirichlet BC)
- eigenstates of quantum particles trapped in a cavity
- acoustic resonances and duct transmission (Neumann BC)
- paradigm for more general trapped wave problems

*e.g.* full Maxwell for microwave, optical resonators

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Modern questions & applications involve…

1. Complex geometry: corners, 3D structures
2. Higher frequencies: *multiscale* problem, $\lambda \ll$ system size

$\boxed{\text{VIEW } j \sim 3000\text{, 45 wavelengths across}}$

# Mathematical questions

1. 'Quantum chaos': what happens in $E \to \infty$ (high freq) limit?
   - depends on classical (ray) dynamics … what if chaotic?
   - arose in quantum physics (Einstein 1917, Gutzwiller, Berry '80s)
   - eigenvalue $E_j$ statistics $\longrightarrow$ Random Matrix Theory
   - physics/chemistry impact: atomic, molecular…

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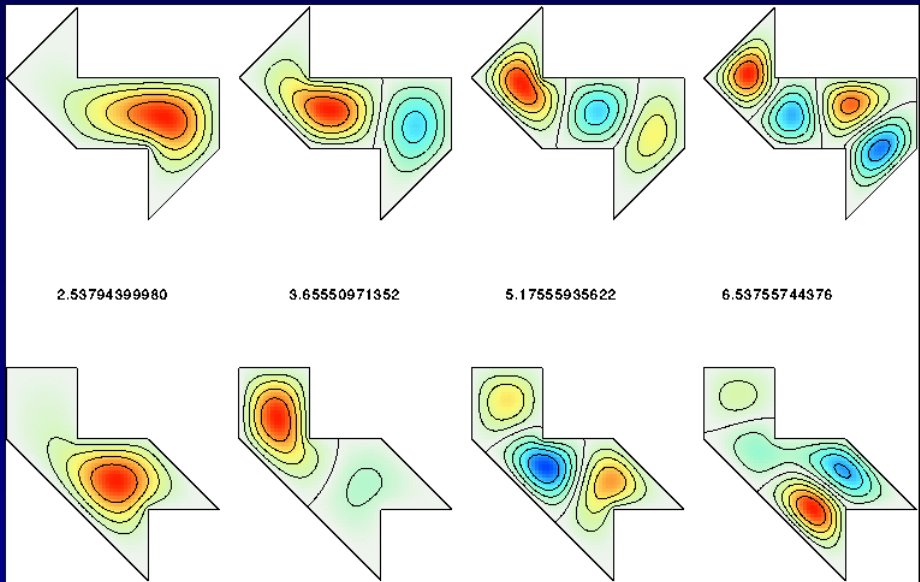
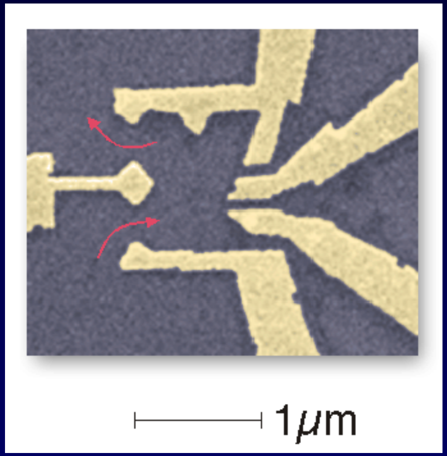
2. Spectral geometry, Riemann surfaces
    - can one hear the shape of a drum? (Kac '66, Gordon *et al.* '92)

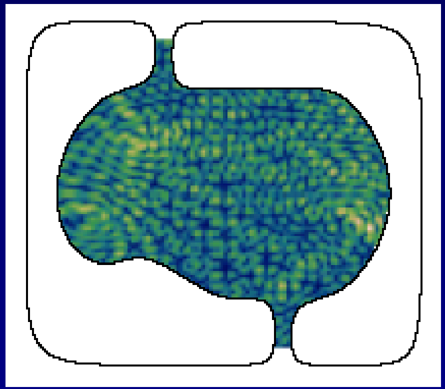


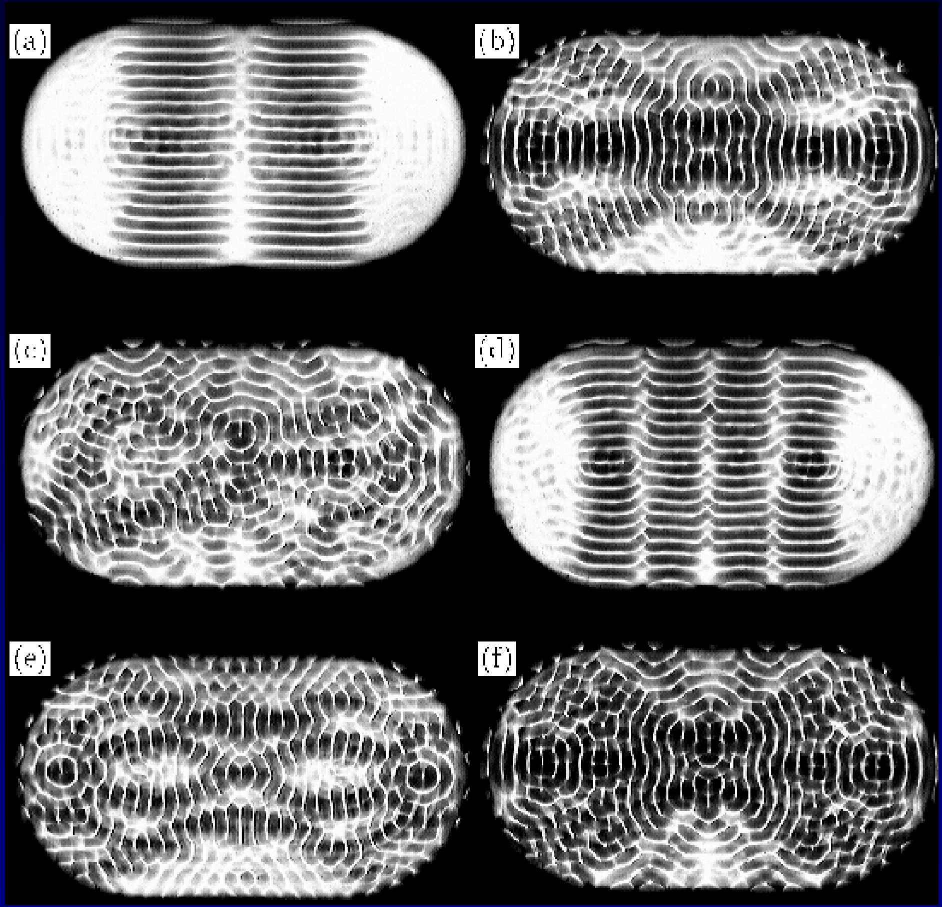

isospectral drums, accurate numerics (Driscoll '97)

# Modern applications

- ‘quantum dots’: $\sim 1\mu$m semiconductor labs for cold electrons
  —candidates for *quantum computers*
  —quantum chaos vital for statistics of resonances, conduction
- waveguide scattering via transverse modes (*e.g.* radar from jet inlets)



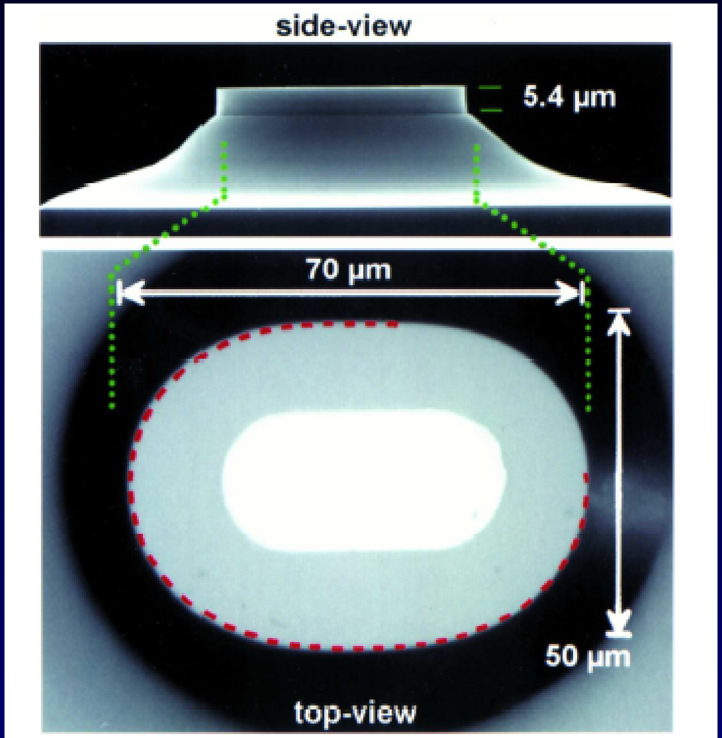



quantum dots (Marcus)

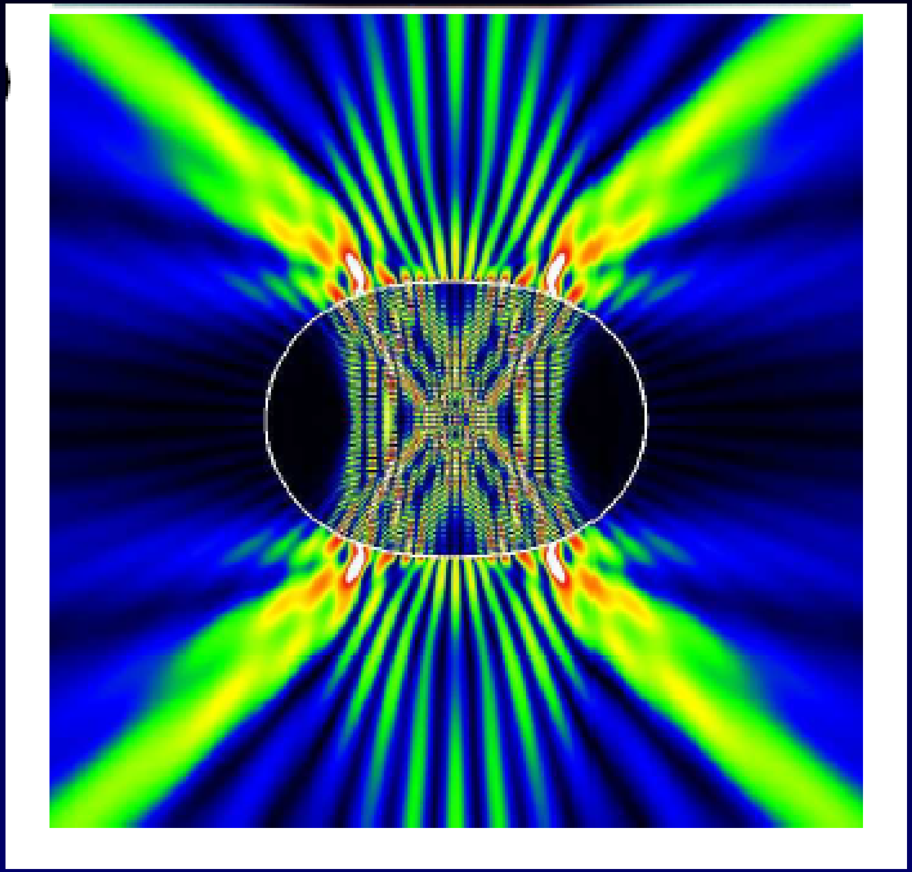
resonant liquid surfaces (Kudrolli)

# Dielectric micro-cavity lasers

quantum-cascade laser




mode and emission pattern



- 2D cavity confinement due to total internal reflection, $n = 3.3$.
- asymmetric cavity, 'scarred' modes $\rightarrow 10^3$ more power (Gmachl '98)
- design is hard: compute many modes for many shapes (Tureci '03)

# Outline

I. modified Method of Particular Solutions

II. eigenvalue inclusion bounds & rigorous analysis

III. acceleration by scaling

IV. application to

- quantum chaos: high-frequency mode asymptotics
- micro-cavity lasers

# I. Modified Method of Particular Solutions (B '00)

Task: find $\phi_j$ and $E_j$ such that $(\Delta + E_j)\phi_j = 0$ and $\phi_j|_{\partial\Omega} = 0$

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- if can find coeff vector $\mathbf{x} \in \mathbb{R}^N$ giving $u|_{\partial\Omega} = 0$, but $u \neq 0$ in $\Omega$

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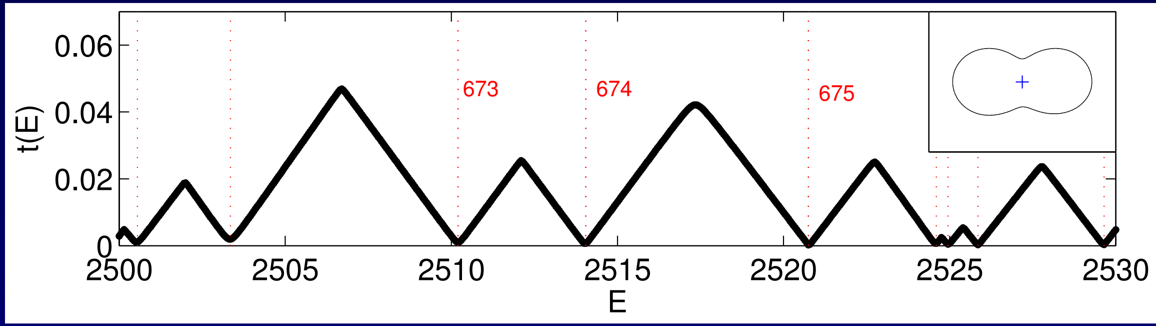
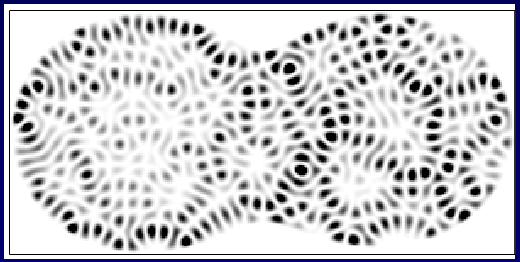



'peanut' cavity, $j \approx 700$



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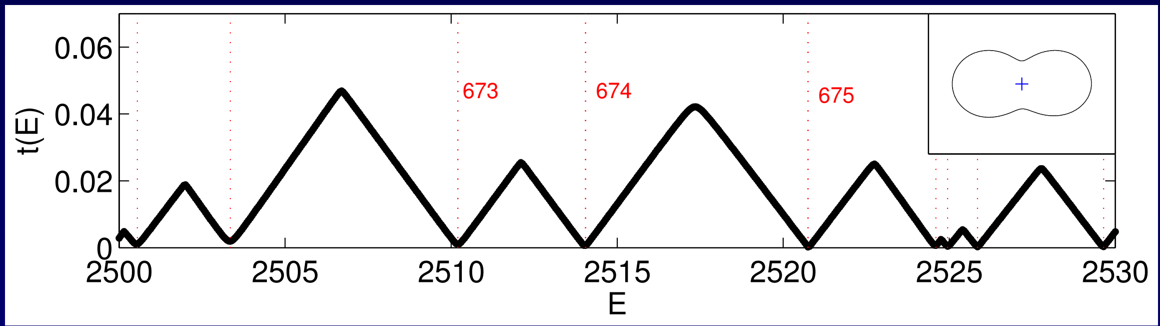


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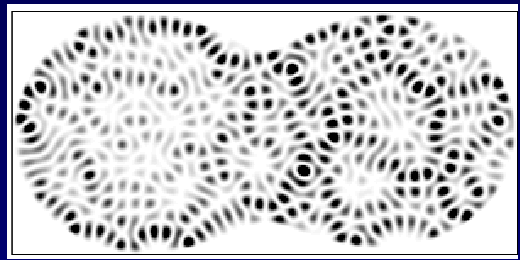

Search (Newton) in $E$ for minima of $t(E)$

- Cures normalization problem plaguing original MPS (Fox '67, etc)

similar cure also recently found (Betcke & Trefethen '04)

# At each $E$, how is $t(E)$ computed?

defining bilinear forms $f(u,v) := \int_{\partial\Omega} uv$ boundary

$g(u,v) := \int_{\Omega} uv$ interior

Rayleigh quotient $t(E) := \min_{u\neq 0} \sqrt{\frac{f(u,u)}{g(u,u)}} = \min_{\mathbf{x}\neq\mathbf{0}} \sqrt{\frac{\mathbf{x}^T F\mathbf{x}}{\mathbf{x}^T G\mathbf{x}}} = \hat{\lambda}_1$

$\hat{\lambda}_1$ = lowest generalized eigenvalue of order-$N$ matrix eigenproblem

$$F\mathbf{x} = \hat{\lambda} G\mathbf{x}$$

elements $F_{ij} := \int_{\partial\Omega} \xi_i \xi_j$ quadrature on boundary (trapezium)

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$F, G$ dense symm positive-definite, numerically singular as $N$ large

- $F, G$ share common nullspace $\rightarrow$ both stable and unstable $\hat{\lambda}$'s
- Cholesky and QZ fail: use *regularized* (truncated) inverse of $G$

# **Basis sets: *global* solutions in $\Omega$**

(cf direct discretization, finite elements: *local* methods)

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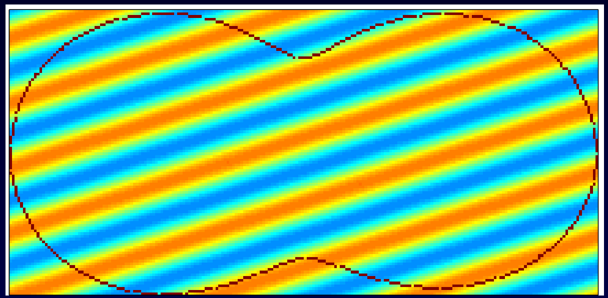
PLANE WAVES



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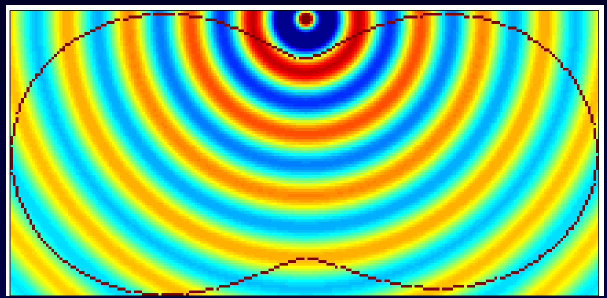
physics community (Heller '84)

FUNDAMENTAL SOLUTIONS



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$\mathbf{y}_i$ on exterior curve (B '02)

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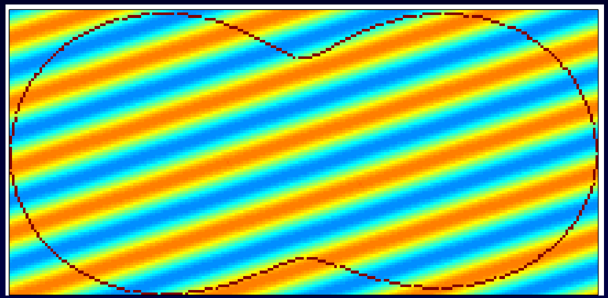

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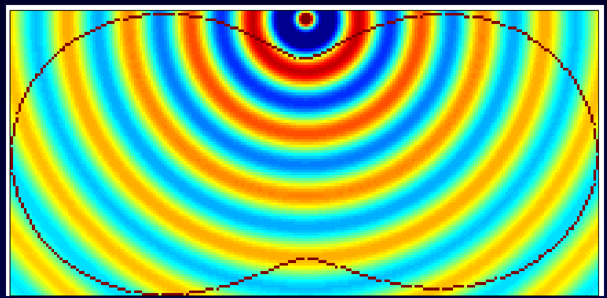

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- Direct discretization: $N \sim$ # wavelengths in volume $\sim k^d$
- We have much smaller $N \sim$ # wavelengths on boundary $\sim k^{d-1}$

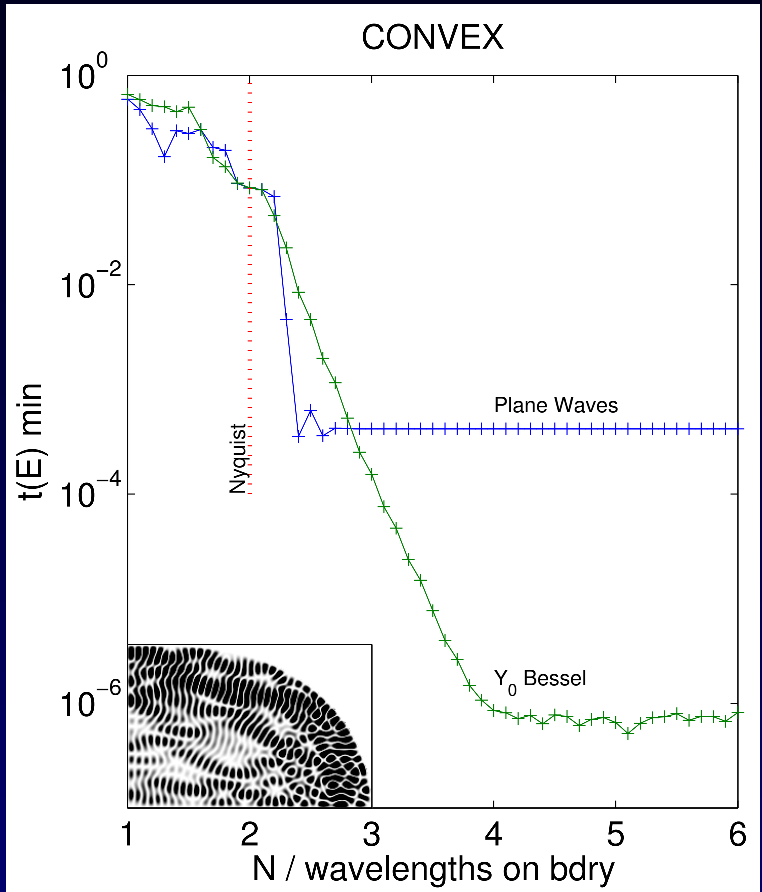
$\Rightarrow$ high frequency : huge advantage (even with loss of sparsity)

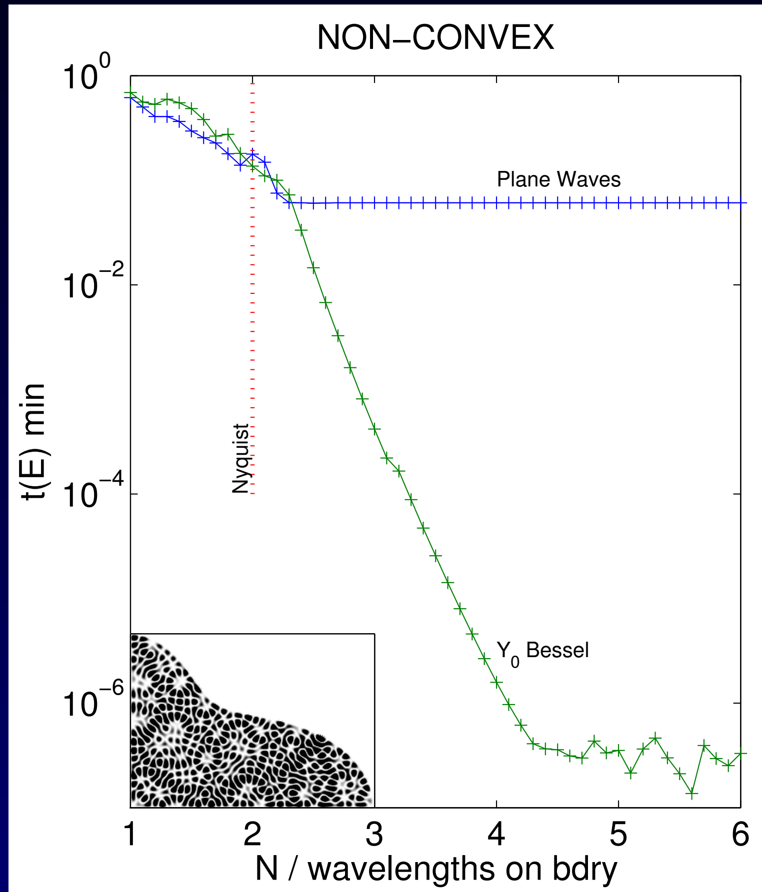
Recall all $\xi_i$ need to be recomputed at each $E$ during search

How compares to boundary integral equation methods / BEM ?

# Convergence with basis size $N$

How small can we make boundary error $t(E)$ ?



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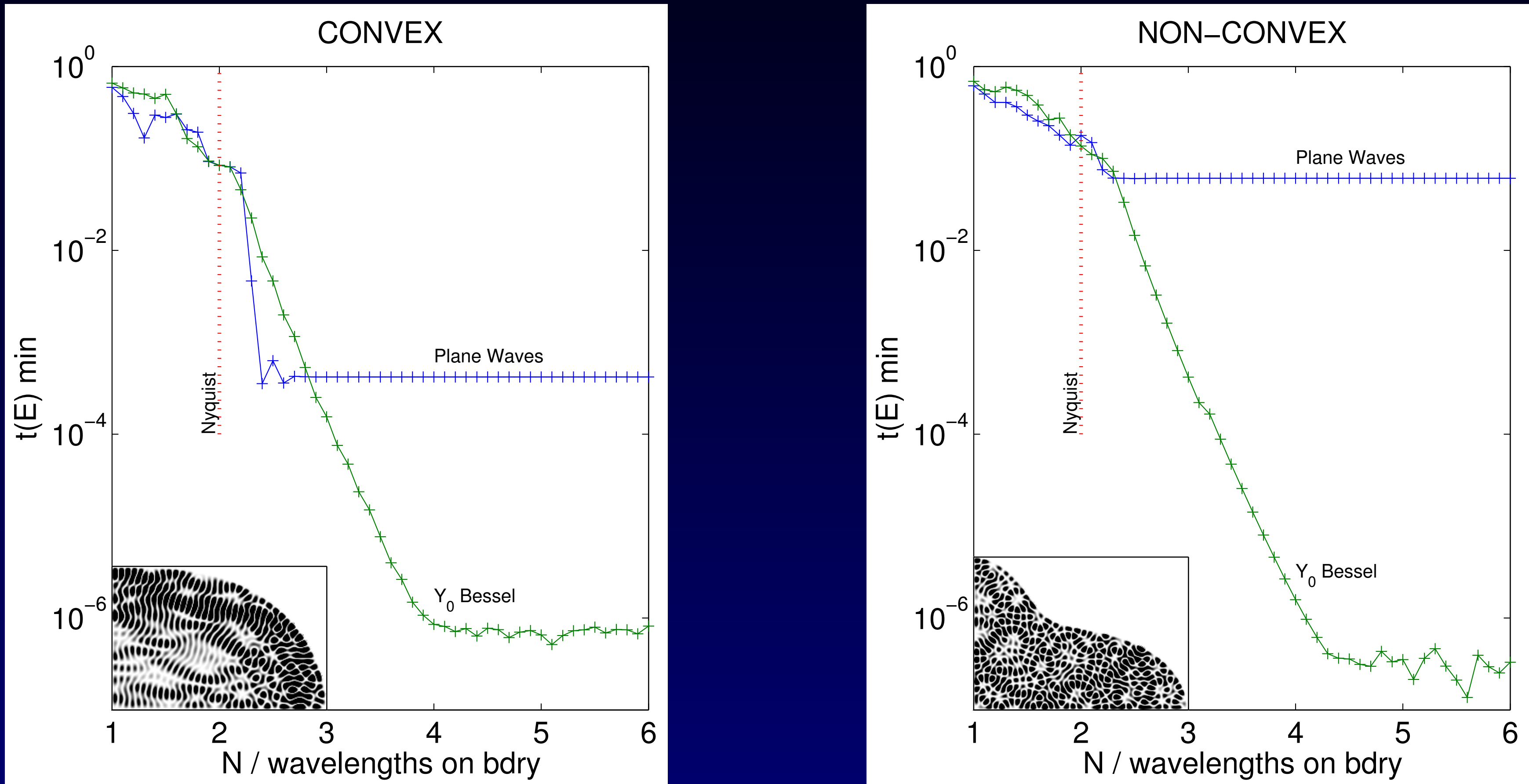


- 3-4 points per wavelength, beats 10 common for integral eqns / BEM
- ‘semiclassical’ basis size $N_{sc}$ = Nyquist limit at spatial frequency $k$
- plane waves useless for non-convex $\Omega$
- Bessels give exponential convergence beyond $N_{sc}$ (down to $\sqrt{\epsilon_{\text{mach}}}$)

# II. Eigenvalue inclusion bounds

Recall $t(E) = \frac{||u||_{L^2(\partial\Omega)}}{||u||_{L^2(\Omega)}}$ for $u$ some global solution $(\Delta + E)u = 0$ in $\Omega$

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Actually can do much better. . .

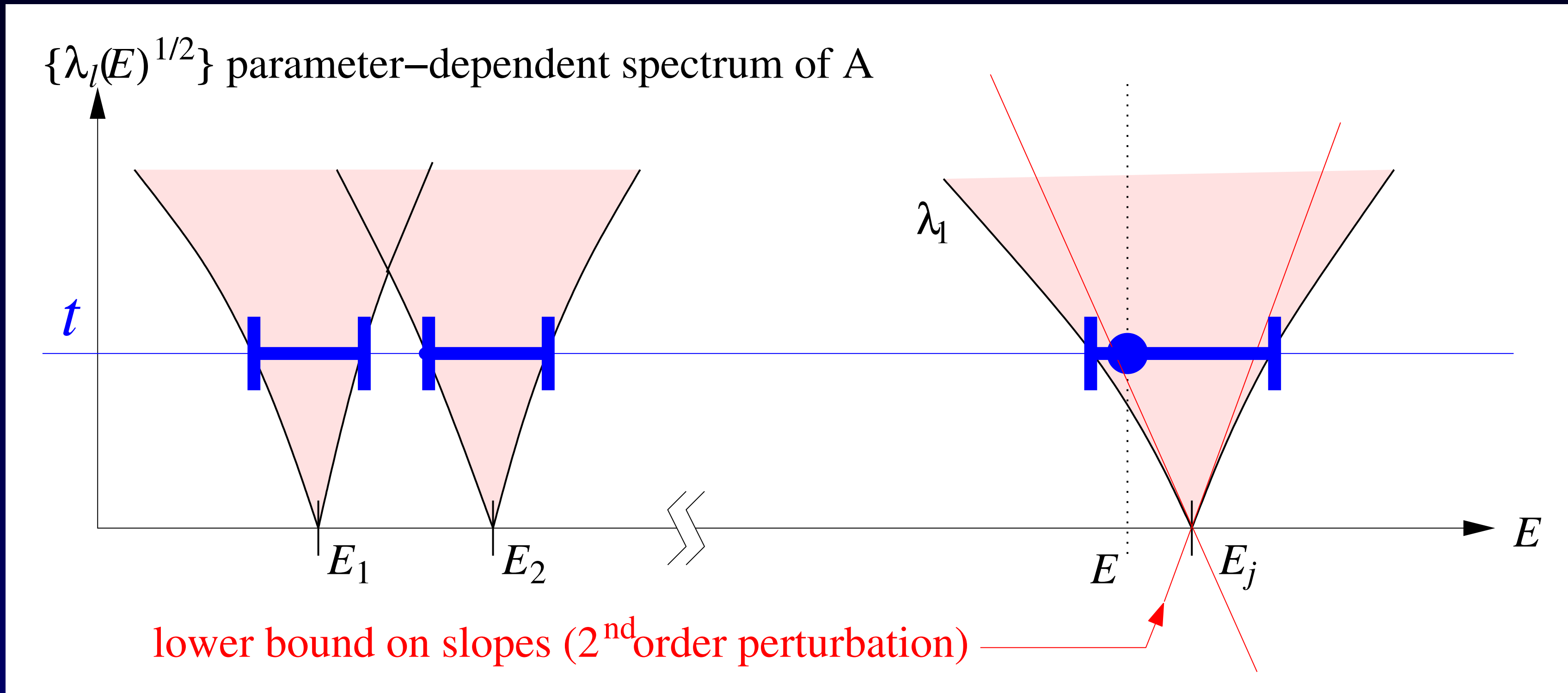
Thm (B '04): For some $\delta$ which vanishes as $t(E) \to 0$,

$$\min_j \frac{|E - E_j|}{E_j^{1/2}} \leq C'_\Omega (1 + \delta) t(E)$$

- In practise $\delta$ is tiny and can be ignored
- High freq $E \sim 10^6$: now $t(E) = 10^{-6}$ means 9-digit accuracy!

# Mechanism for improved inclusion

For all $E$: $t(E)^2$ exceeds lowest eigenvalue $\lambda_1(E)$ of an operator $A(E)$



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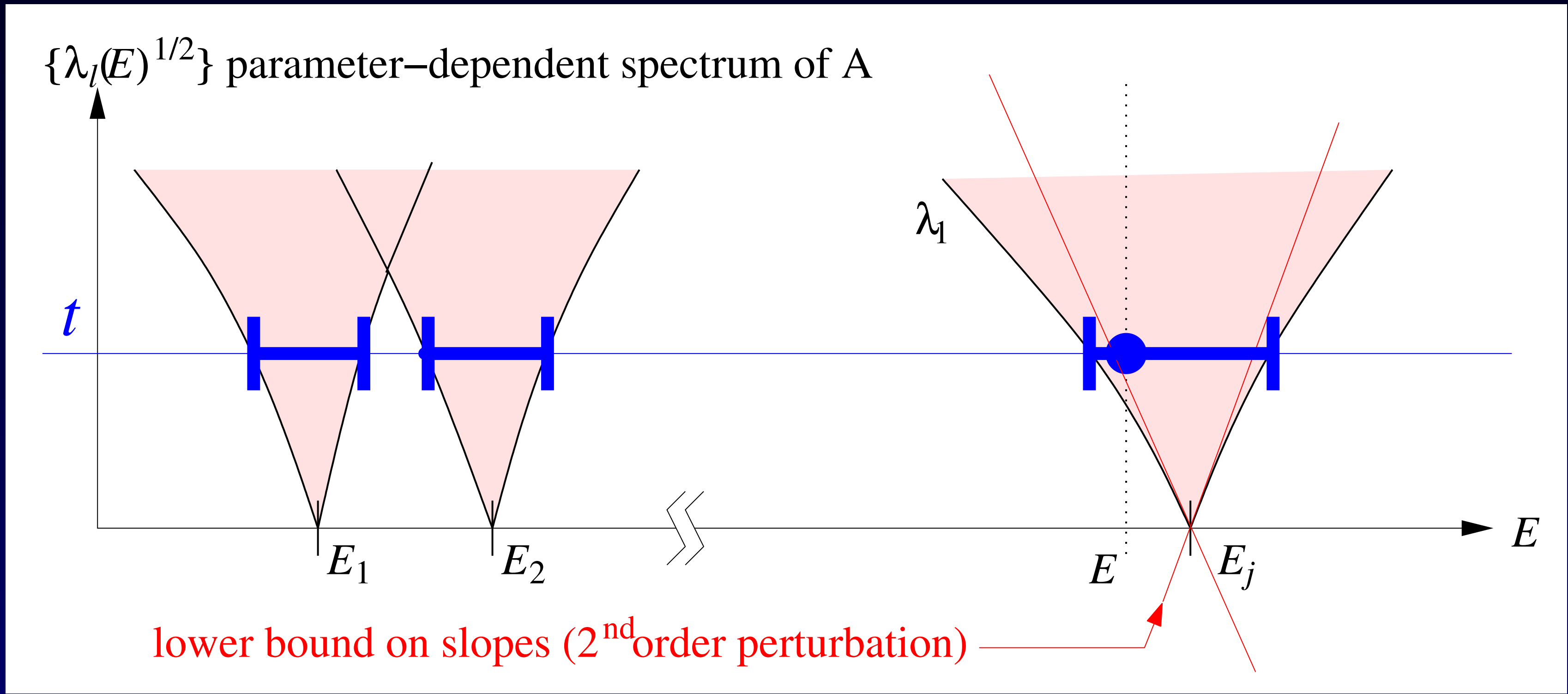


prove analytic perturbation series $\lambda_1(E) = c_j(E - E_j)^2 + O(E - E_j)^4$

- so as $t \to 0$, error $|E - E_j|$ must vanish like $c_j^{-1/2} t$
- 'slope' coefficients $c_j$ bounded from below by $c/E_j$, for all $j$

# Rigorous analysis (sketch) (w/ Deift, Goodman)

Work in $\infty$-dim space $\mathcal{H}_\Omega(E) := \{(\Delta+E)u=0 \text{ in } \Omega,\ u|_{\partial\Omega}\in L^2(\partial\Omega)\}$

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Finally, note $t(E)^2 = \hat{\lambda}_1 \ge \lambda_1$ since $\text{Span}\{\xi_i\} \subset \mathcal{H}_\Omega(E)$

RESULT: new inclusion bounds, tighter by factor $E^{1/2}$

# III. Acceleration by scaling

(back to numerical method, $N$-dim Span$\{\xi_i\}$)

Root search slow, close levels easily missed — can we do better?

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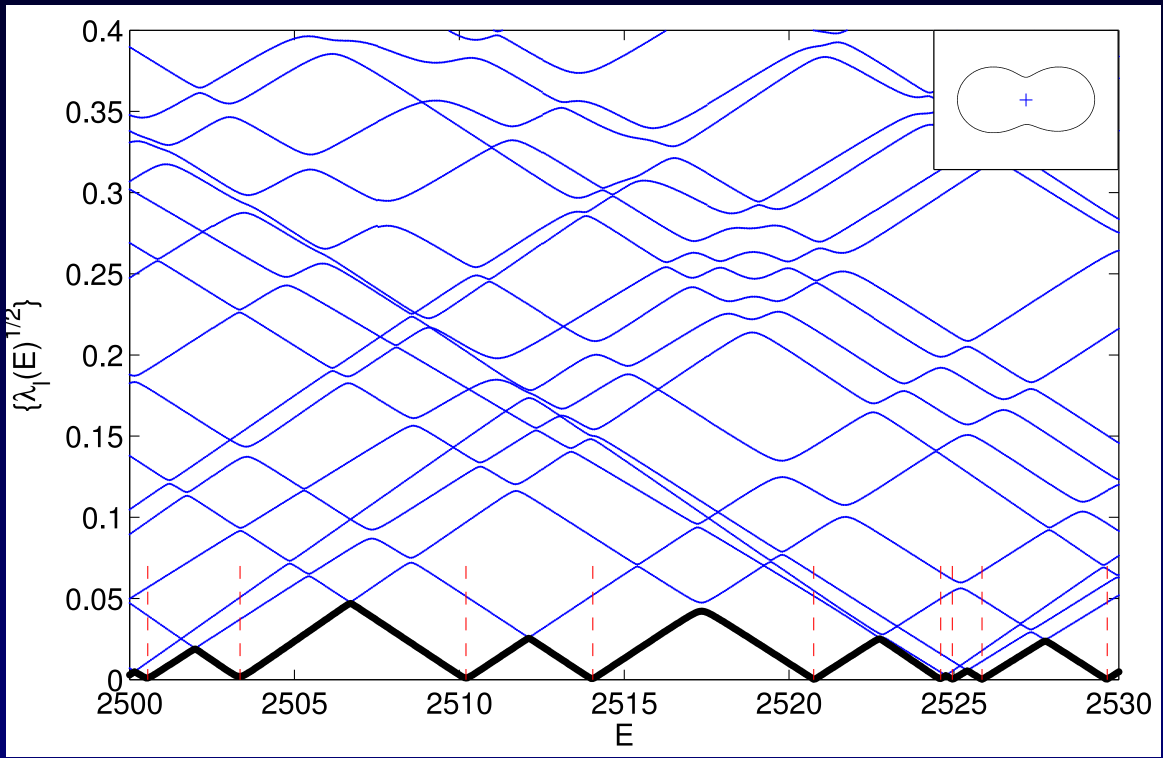

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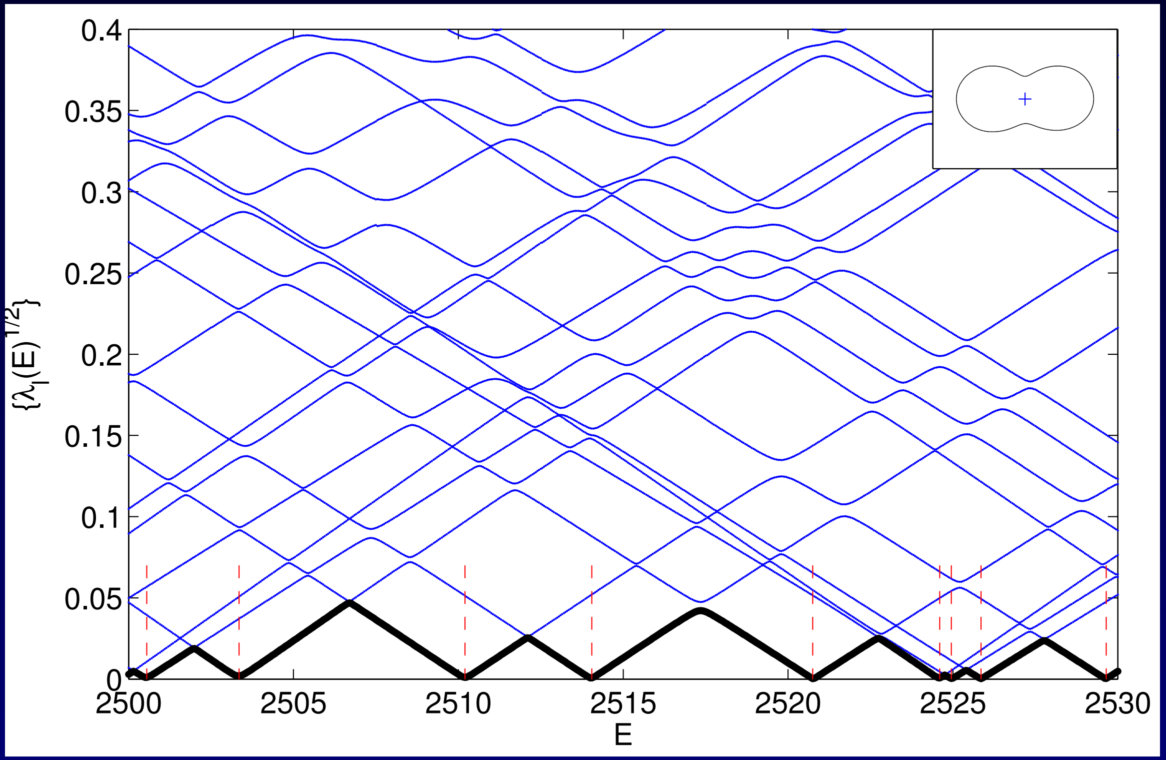


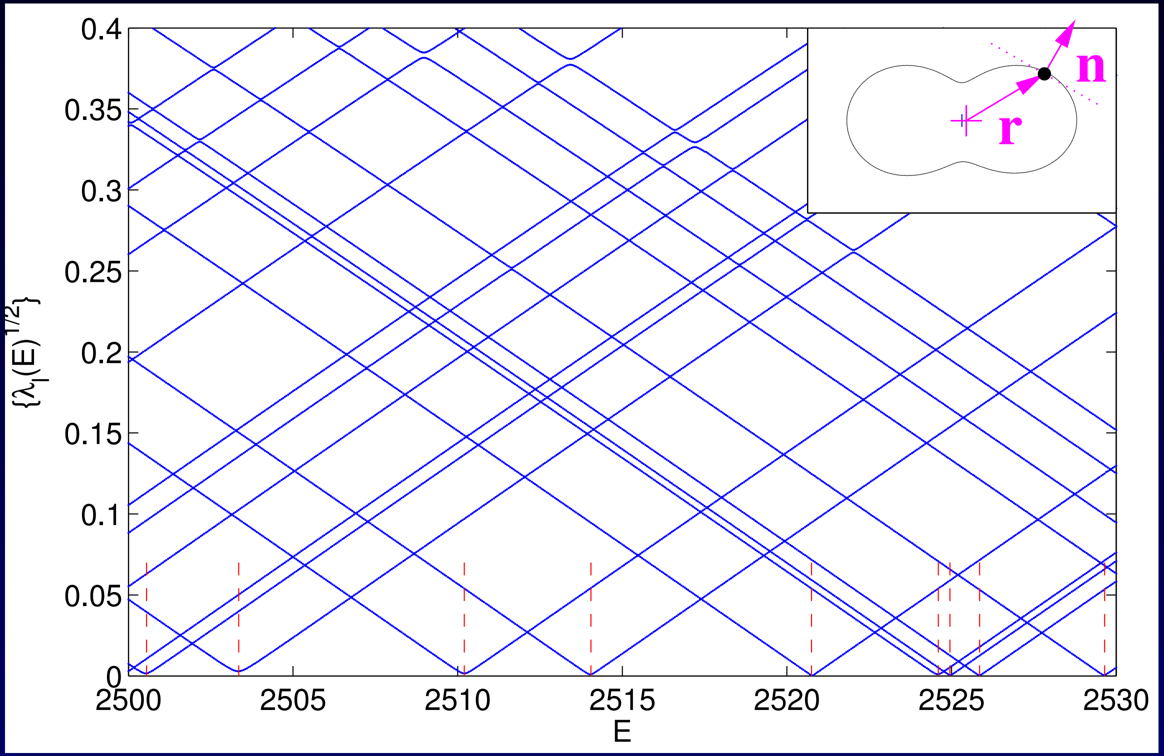

- Idea: spectrum at single $E$ has info about many nearby $\hat{\lambda}_1$ minima

# Special boundary weighting $w$

For $f$, change from $w = 1$ to $w = (\mathbf{r} \cdot \mathbf{n})^{-1}$ (requires $\Omega$ star-shaped)

# Special boundary weighting $w$

For $f$, change from $w = 1$ to $w = (\mathbf{r} \cdot \mathbf{n})^{-1}$ (requires $\Omega$ star-shaped)




- spectacular: beautiful quadratic structure, tiny avoided crossings
- no variation in $2^{nd}$-order coeffs $\longrightarrow$ accurate predictive power!

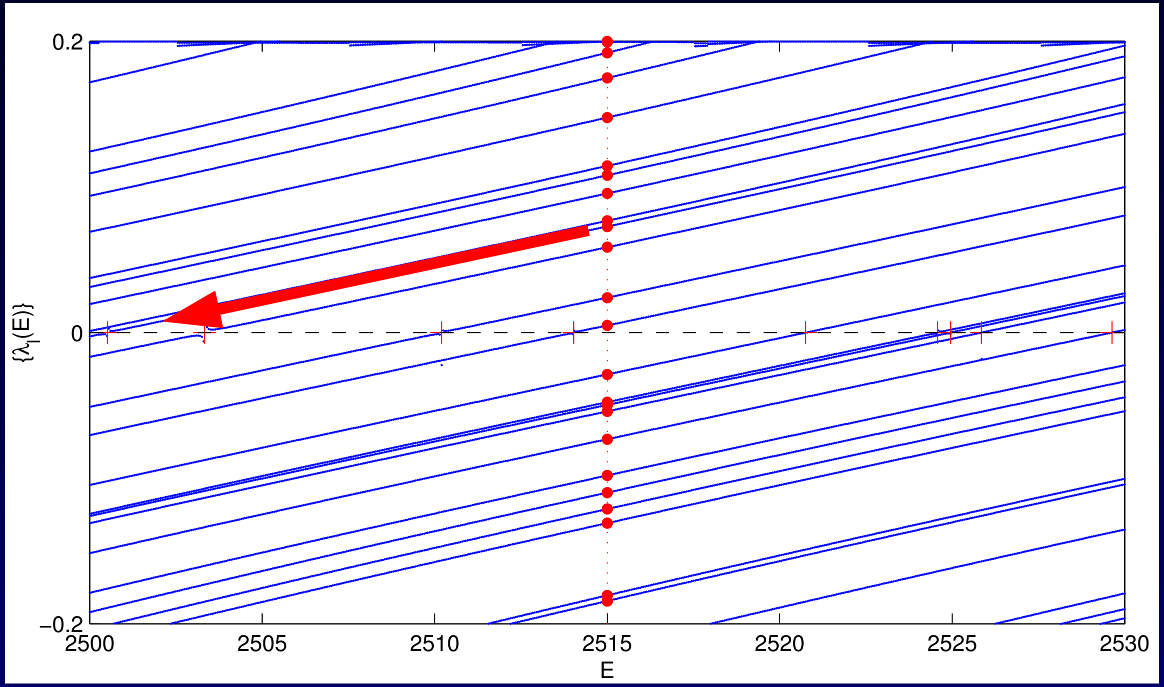
But we can do even better. . .

# Scaling method

(Vergini '94, B '00, '04)

Invented in physics community... a correct explanation was sorely lacking!

Use $f$ as before, but $g(u,v) = \int_{\partial\Omega} (\mathbf{r}\cdot\mathbf{n})^{-1}(u\mathbf{r}\cdot\nabla v + v\mathbf{r}\cdot\nabla u)$




- solving $F\mathbf{x} = \hat{\lambda} G\mathbf{x}$ at single $E$ value gives all nearest $O(N)$ modes
- no root search, no missing levels, efficiency gain $O(E^{\frac{d-1}{2}})$, in 3D too
- eigenvectors $\mathbf{x}$ give *dilated* (scaled) approximations to modes $\phi_j$
- errors grow like $t \sim |E_j - E|^3$ ($3^{rd}$-order convergence with effort)

# Scaling relies on quasi-orthogonality

modes exactly orthogonal in interior $\int_\Omega \phi_i \phi_j = \delta_{ij}$

approx orthogonality on boundary $Q_{ij} := \int_{\partial\Omega} \mathbf{r} \cdot \mathbf{n} \, \partial_n \phi_i \, \partial_n \phi_j$

It's known $\quad Q_{ij} = 2\delta_{ij} E_j + q_{ij} \quad$ with $q_{jj} = 0$ (Rellich '40)

- conjecture (Vergini '94): off-diag terms grow $|q_{ij}| \sim |E_i - E_j|$
- semiclassics (B-Cohen-Heller '00): for $\Omega$ ergodic, $|q_{ij}| \sim (E_i - E_j)^2$

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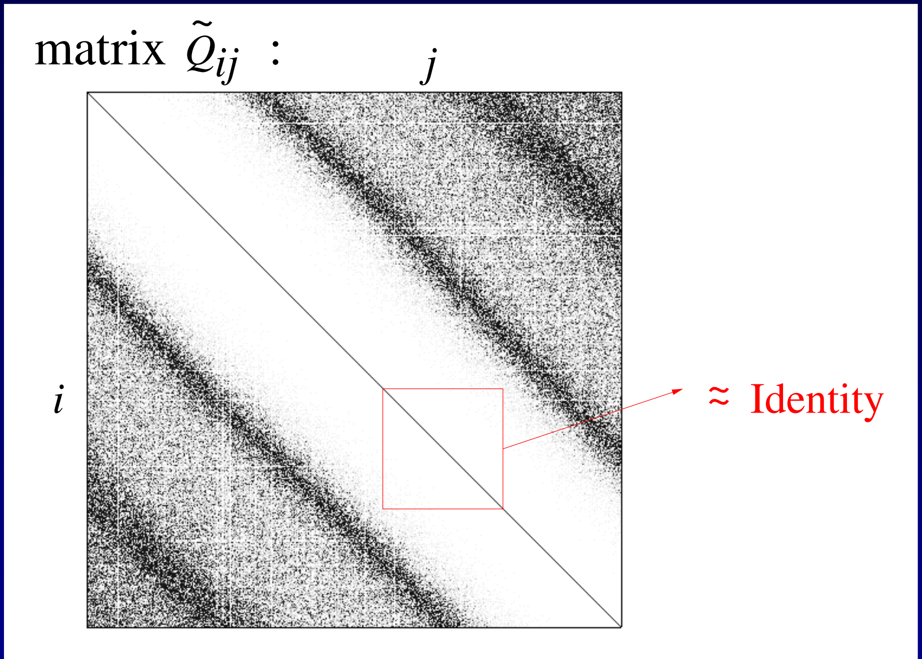
- Thm (B '04): for *all* $\Omega$, ergodic or not, $|q_{ij}| \le C_\Omega (E_i - E_j)^2$




Now can show dilated $\phi_j$ approx diagonalize $f$ and $g$
$\Rightarrow$ scaling works

# VI. Applications

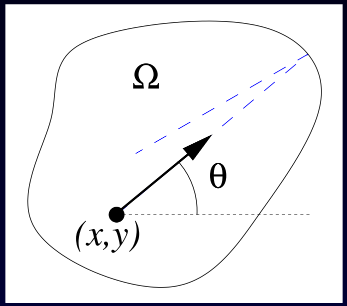
- ‘quantum chaos’: asymptotics of modes in chaotic cavities
- laser cavity modeling

# Quantum chaos & cavity shape

Drum problem is *quantized* equivalent of ‘billiards’

dynamical system: point particle, elastic reflection from $\partial\Omega$

phase space $= (x, y, \theta)$



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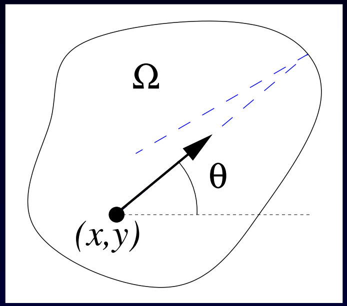


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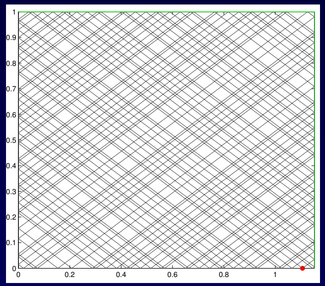
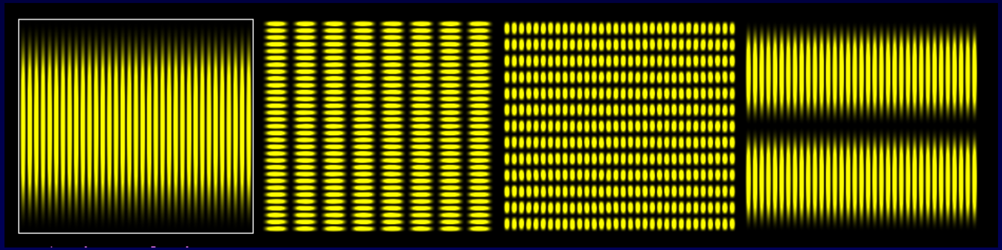
classical    eigenfunctions $\phi_j$: ‘quantum’

Integrable:

conserved quantities

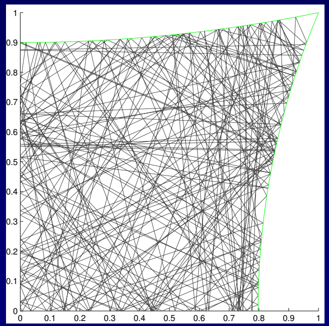


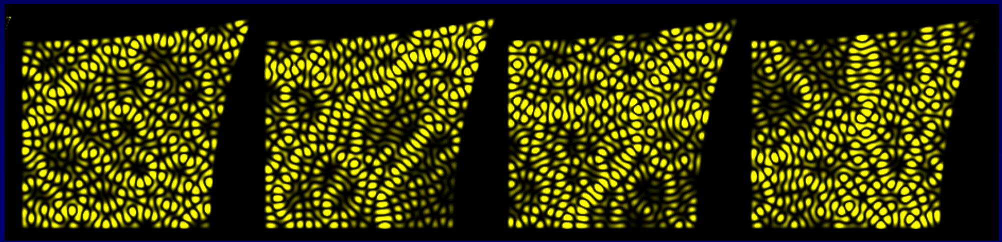


localization (tori in phase space: EBK)

Ergodic:

covers all phase space





‘quantum chaos’

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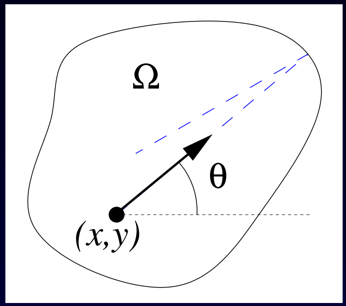


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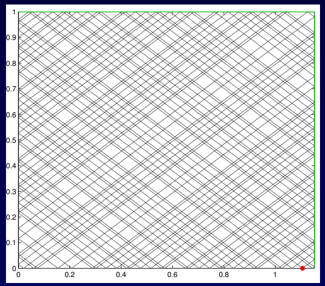

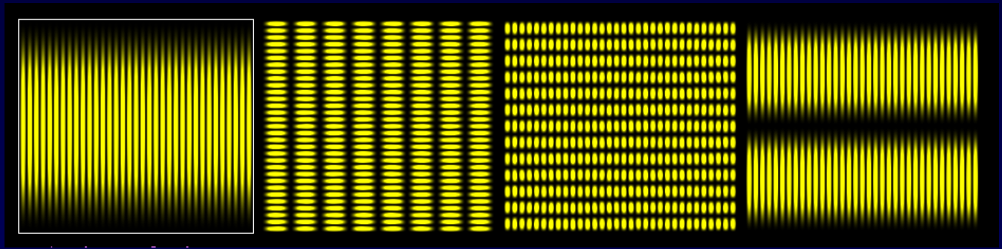

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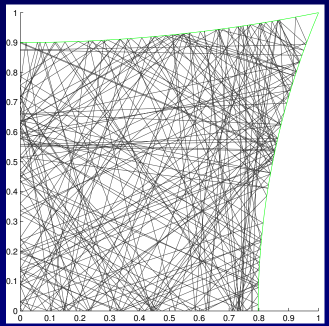
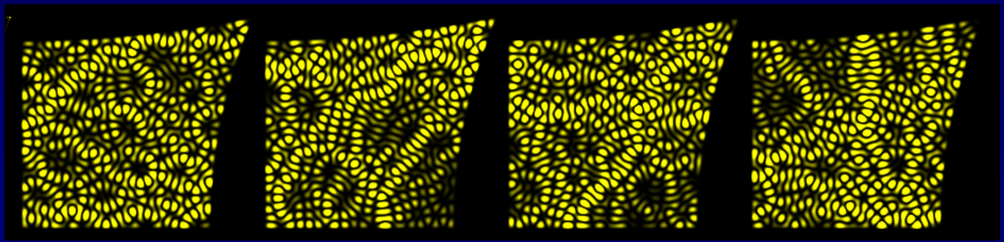




‘quantum chaos’

- We examine mode intensity $\phi_j^2$ for ergodic $\Omega$ in $E \to \infty$ limit

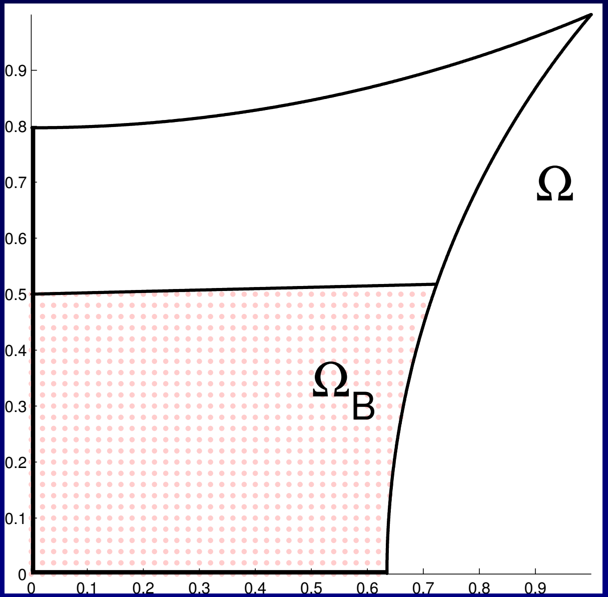
# Do modes become spatially uniform?

Quantum Ergodicity Theorem: For ergodic cavity $\Omega \supset \Omega_B$,

$$\lim_{E_j \to \infty} \int_{\Omega_B} \phi_j^2 = \frac{\mathrm{vol}(\Omega_B)}{\mathrm{vol}(\Omega)} \qquad \text{for 'almost all' } j$$

(Schnirelman '74, Colin de Verdière '85, Zelditch '87, Z-Zworski '96)

But no prediction of convergence rate or density of exceptional set



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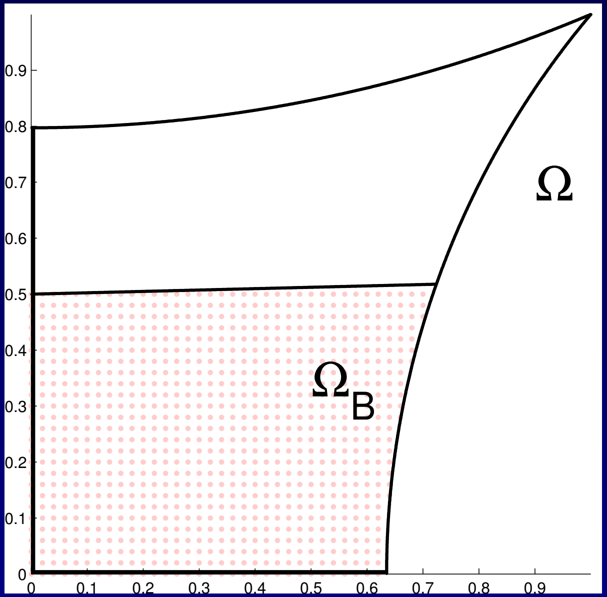
But no prediction of convergence rate or density of exceptional set

Study $\int_{\Omega_B} \phi_j^2 - \mathrm{vol}(\Omega_B)/\mathrm{vol}(\Omega)$ numerically:

- Sinai-type cavity (uniformly hyperbolic)
- 30,000 modes, level numbers $j \sim 10^4$ to $10^6$

  ... 100 times higher than other studies
- only a few CPU-days total (B '04)



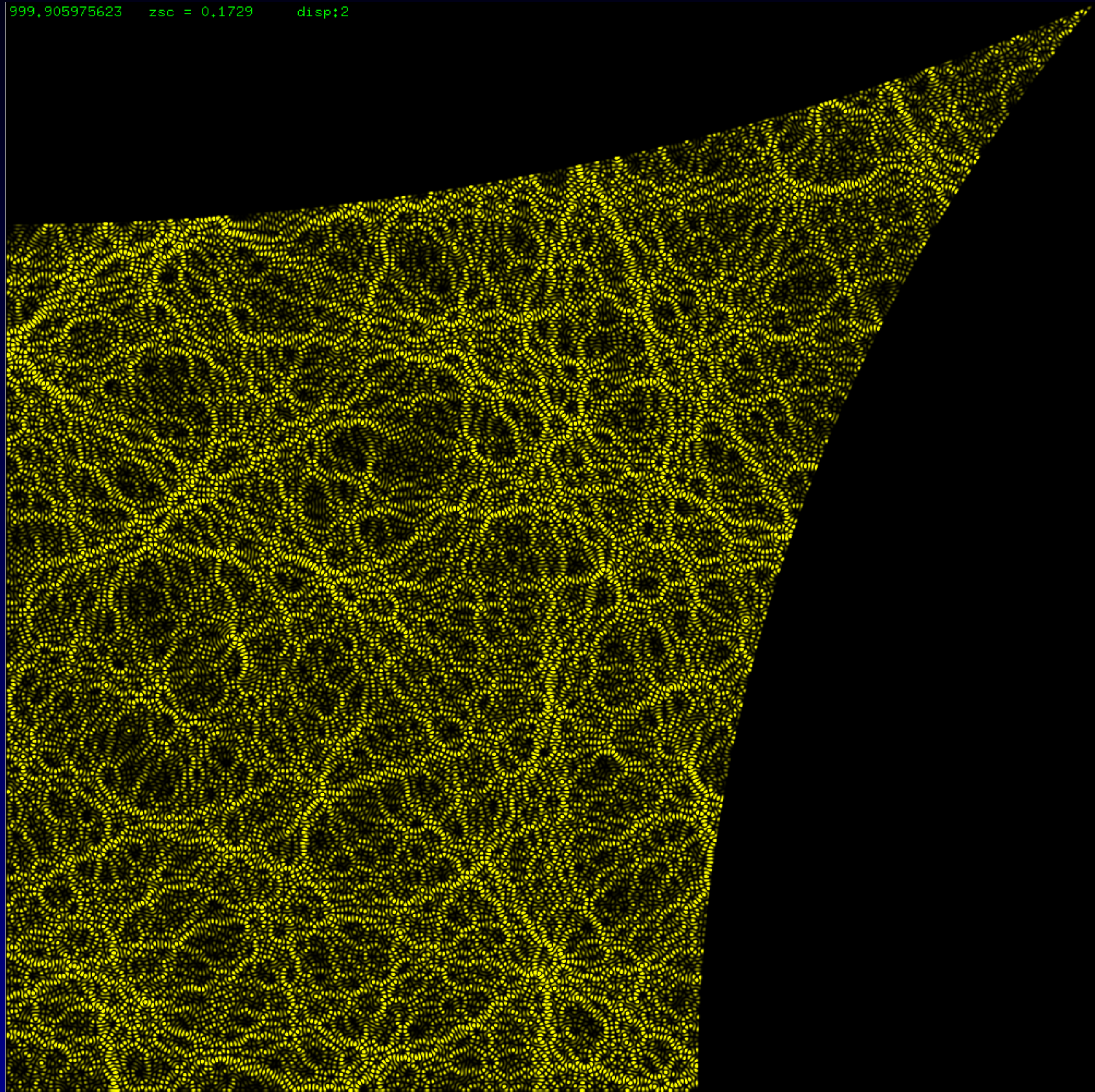
# High-frequency mode

225 wavelengths across system

level number
$j \approx 5 \times 10^4$

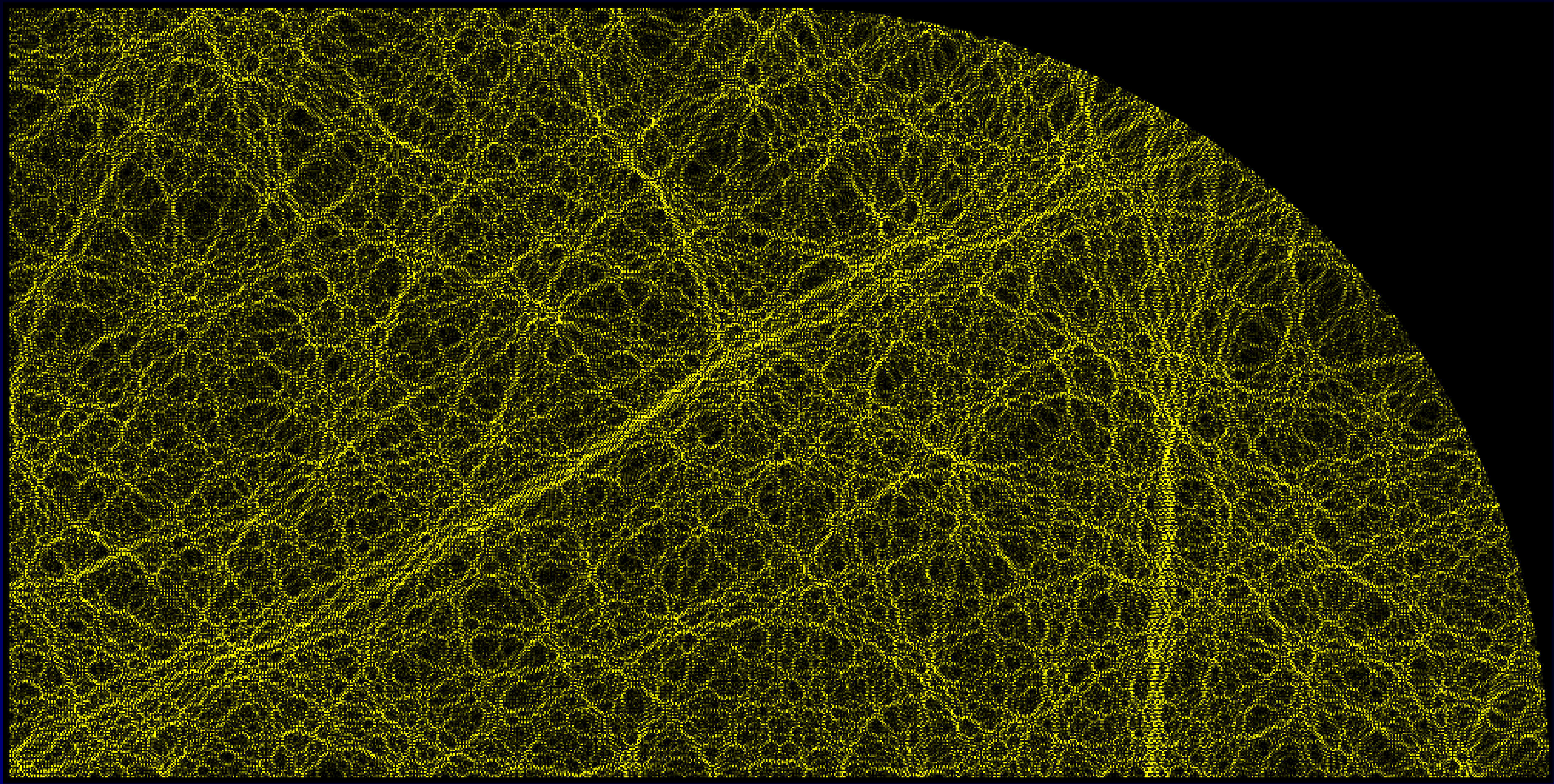
$E \approx 10^6$

here scaling method is $10^3$ times faster than MPS! (or BEM)



# Scarred mode (stadium cavity)

'Scar' is: enhanced intensity $\phi_j^2$ on unstable periodic (ray) orbit



- discovered in physics, predict width dies $E \sim E^{-1/4}$ (Heller '84)

# Result: asymptotic convergence rate with $E$

local variance $$V_B(E) := \frac{1}{E^{1/2}} \sum_{E_j \in [E, E+E^{1/2}]} \left( \int_{\Omega_B} \phi_j^2 - \frac{\mathrm{vol}(\Omega_B)}{\mathrm{vol}(\Omega)} \right)^2$$

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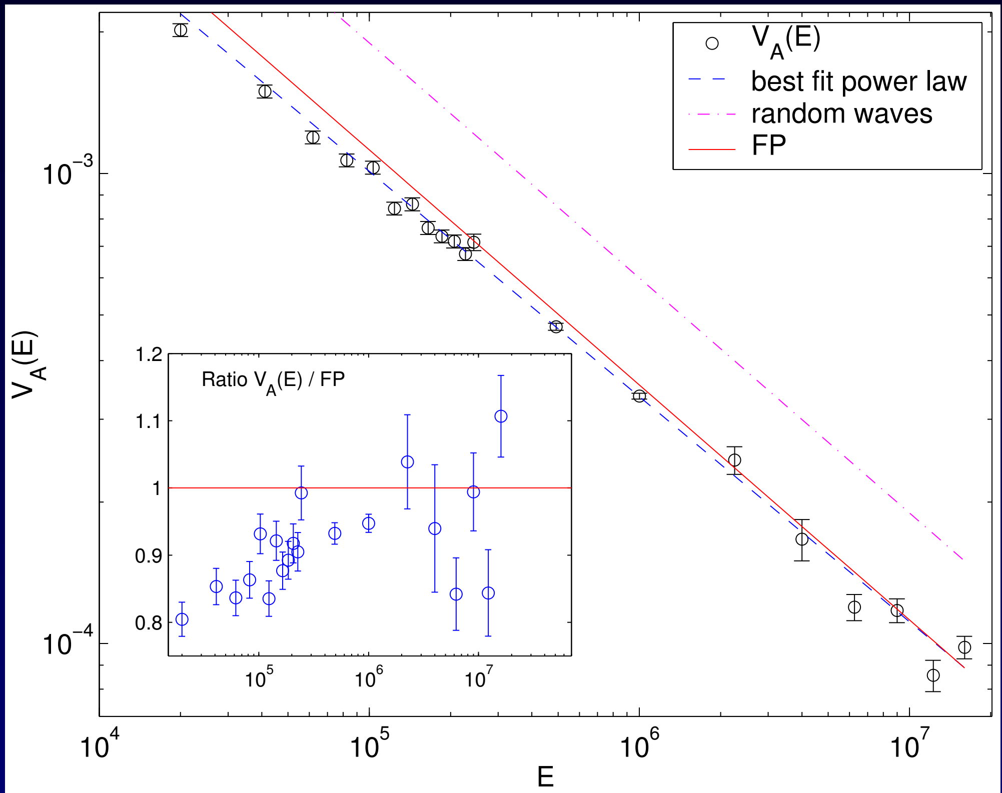


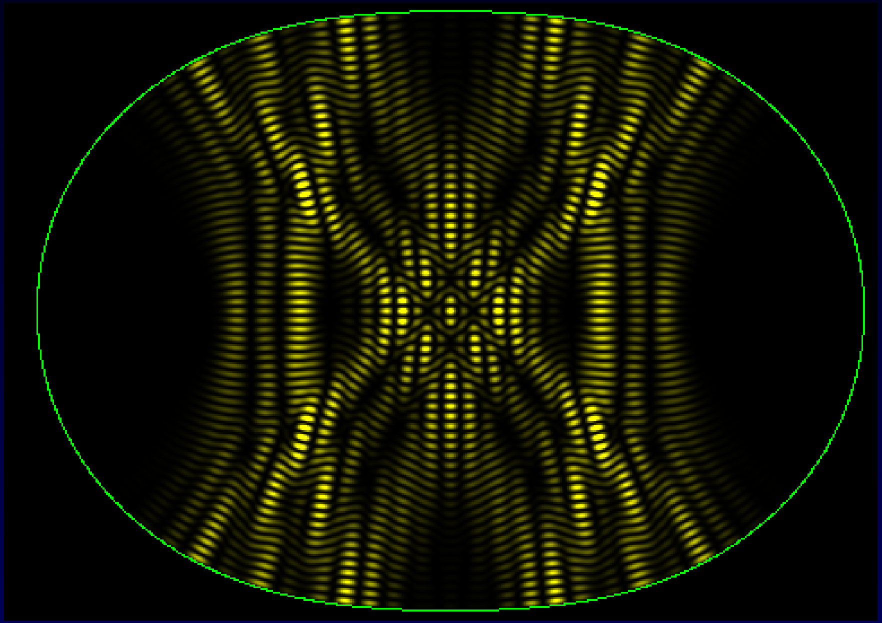

consistent with power law model $V_B(E) = aE^{-\gamma}$

fit $\gamma = 0.48 \pm 0.01$

- large numbers of modes $\longrightarrow$ highly accurate statistics ($< 1\%$)
- rate agrees with semiclassical results and scar theory $\gamma = 1/2$
- no exceptional modes: supports Quantum Unique Ergodicity (Sarnak *et al.* )

# Laser results: closed cavity modes

$E = 16417.2$ MODES

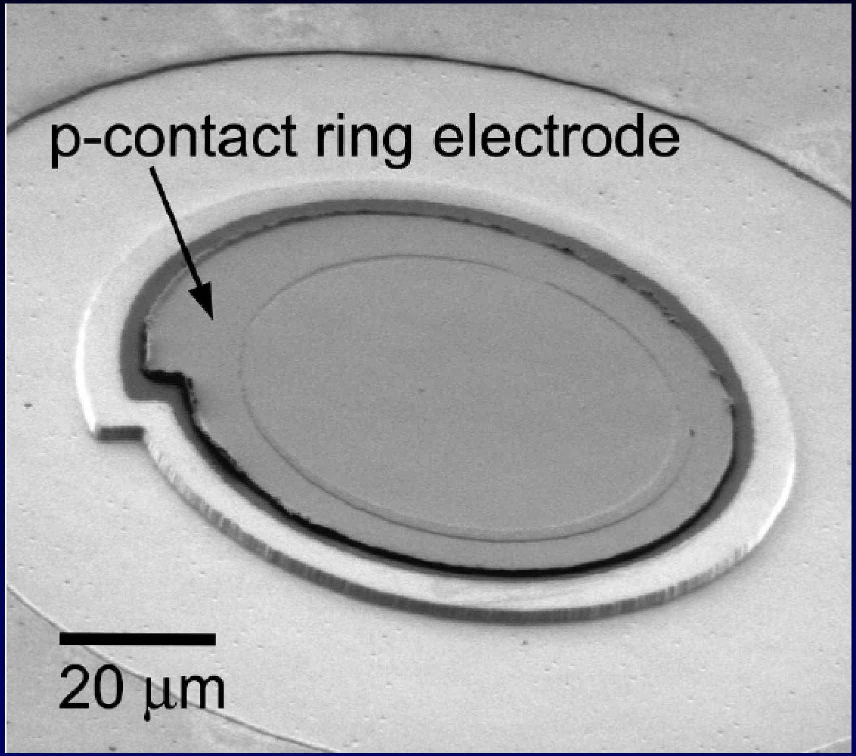


| CPU / mode | method |
|---|---|
| 60 s | MPS, root search |
| 10 s | scaling, $\phi_j$ across $\Omega$ |
| 0.6 s | scaling, $\phi_j$ bdry only |

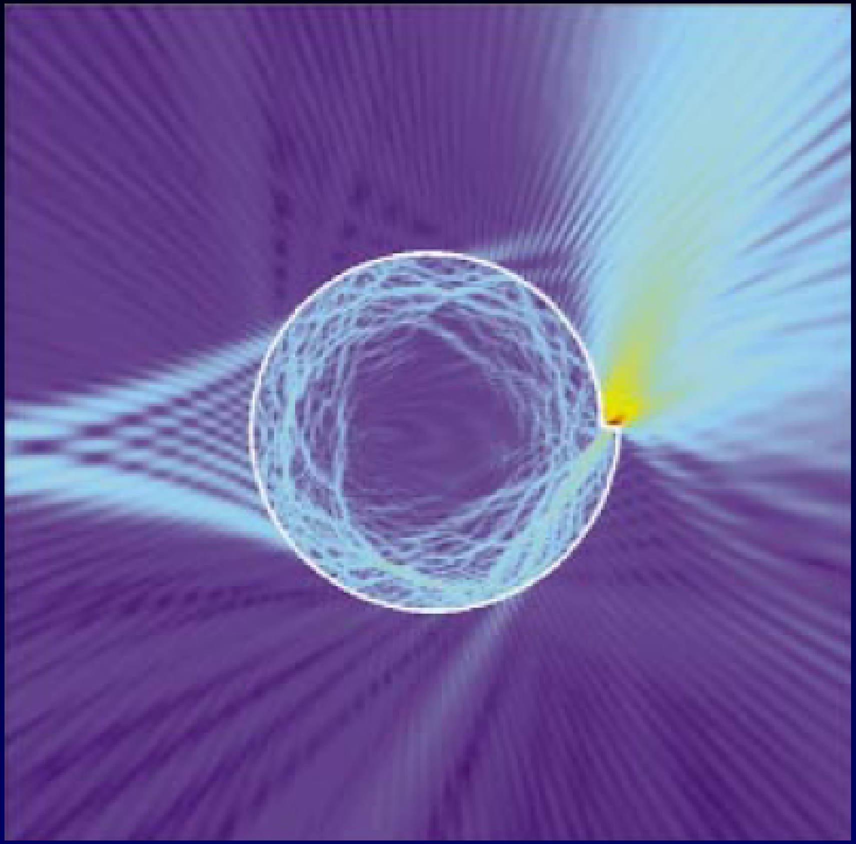
Ongoing with Hakan Tureci (Yale):

- mode evolution equations need integrals $\int_\Omega \phi_i^2 \phi_j^2$
- open mode lifetime and emission via perturbation theory in $1/n$

# Future laser plans: spiral cavity




micrograph (Kneissl *et al.* ’04)

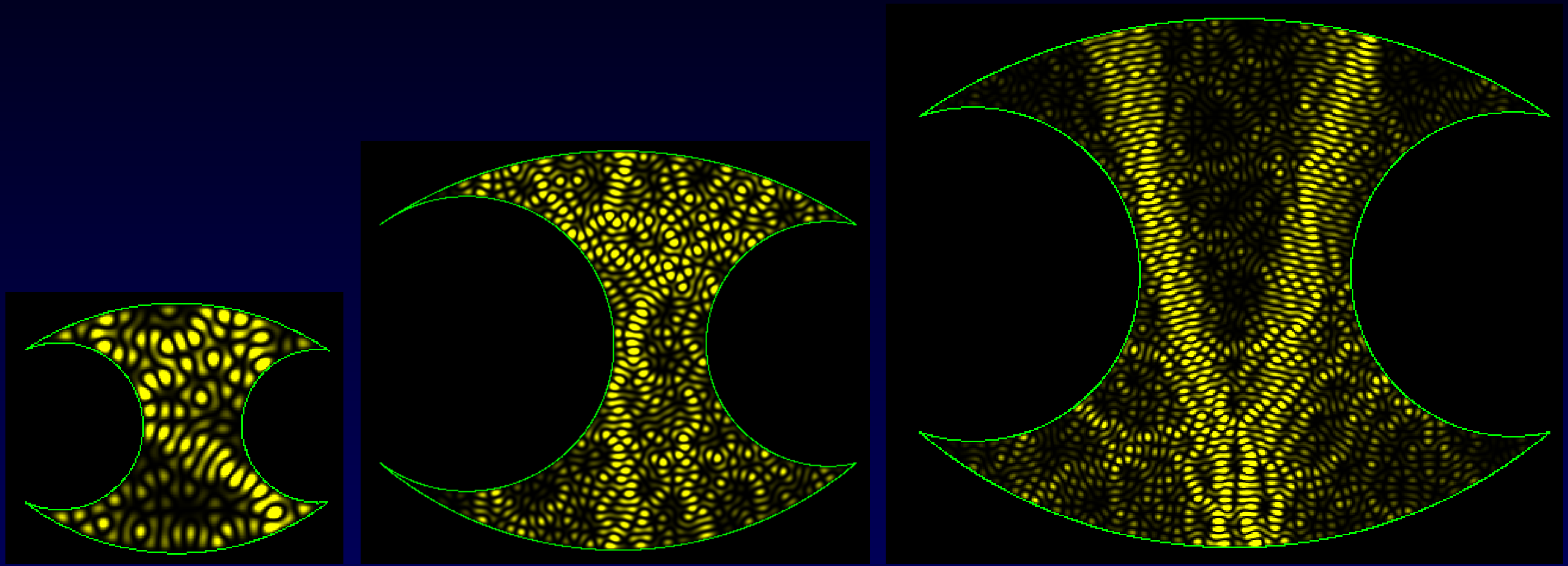


numerics (Chern *et al.* ’03)

- what optimal shapes?
- where best to pump (spatially)?
- so far computations hard & limited in wavenumber

# Non-star-shaped domains: initial results

Boundary weight $w = 1/(\mathbf{r} \cdot \mathbf{n})$ no longer bounded nor positive



- scaling method *still works*: not great accuracy, $t \sim 10^{-2}$.
- promising for complex geometries. . .

# Conclusions

Dirichlet eigenproblem: global (meshless) methods excel

At high frequencies *e.g.* $\sim 100$ wavelengths across...

- made eigenvalue inclusion $10^3$ times more accurate
- scaling: $10^3$ faster computation than any other known method

Future:

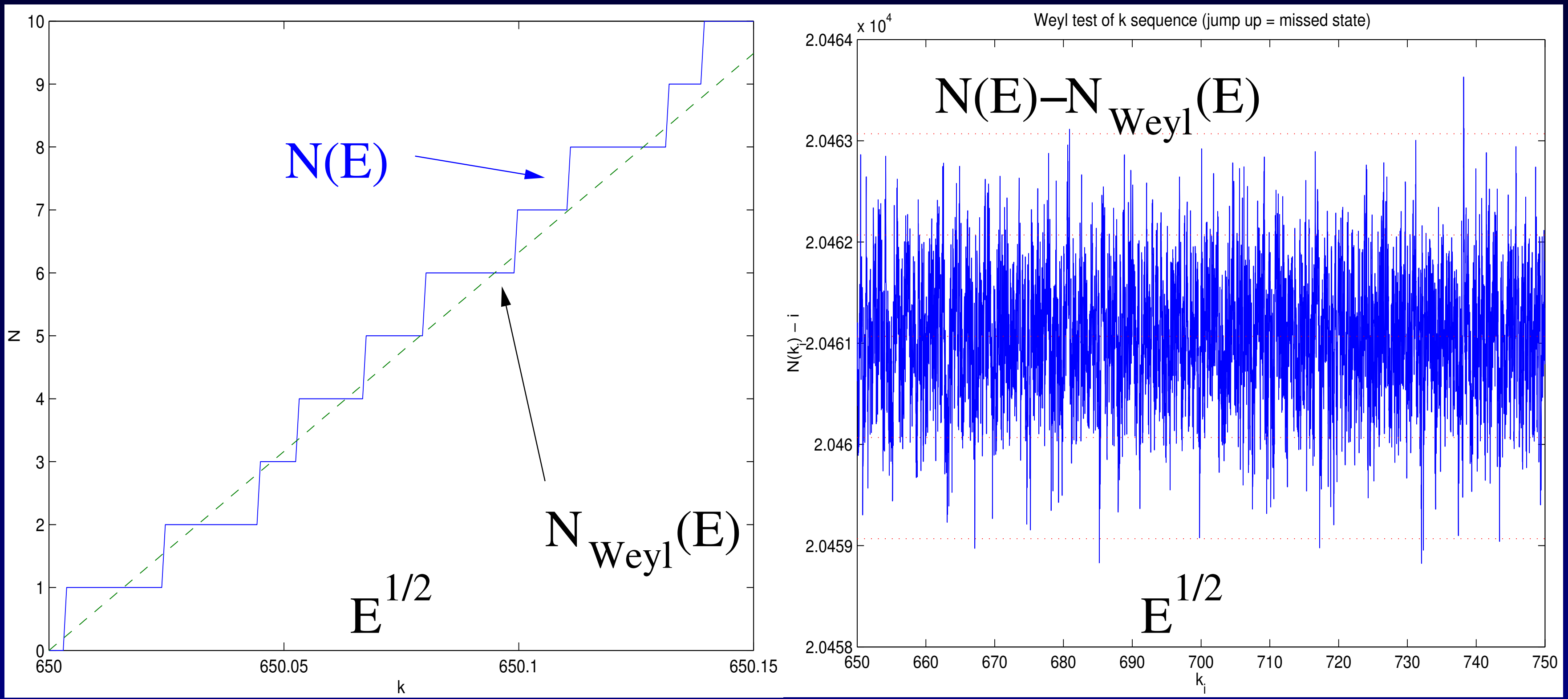
- wider class of cavity shapes, boundary conditions
- rigorous analysis of scaling errors
- accelerate integral equation methods: open problems

Preprints/talks: http://www.cims.nyu.edu/~barnett

# Missing levels?

Weyl's estimate for $N(E)$, the # eigenvalues $E_j < E$:

$$N_{\mathrm{Weyl}}(E) \;=\; \frac{\mathrm{vol}(\Omega)}{4\pi}E - \frac{L}{4\pi}\sqrt{E} + O(1)\cdots$$




- not one level missing in sequence of 6812